



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2017 – 04:44 PM EDT

PDB ID : 1XNS  
Title : Peptide trapped Holliday junction intermediate in Cre-loxP recombination  
Authors : Ghosh, K.; Lau, C.K.; Guo, F.; Segall, A.M.; Van Duyne, G.D.  
Deposited on : 2004-10-05  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

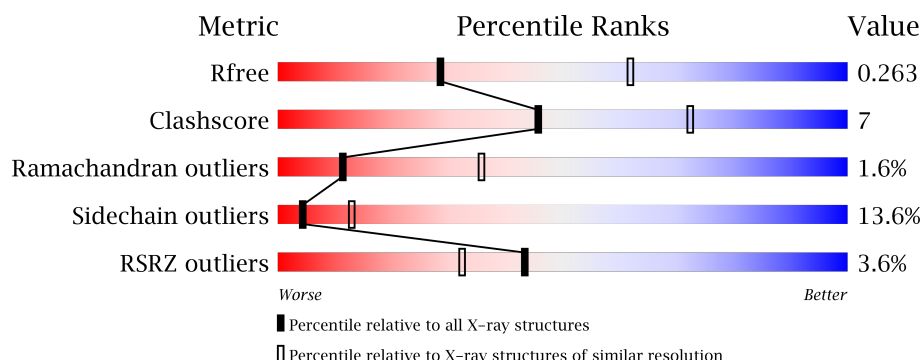
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	35	<div> <div>11%</div> <div>23% 51% 23%</div> </div>
2	D	34	<div> <div>21% 47% 32%</div> </div>
3	A	324	<div> <div>4%</div> <div>71% 24% 5%</div> </div>
3	B	324	<div> <div>3%</div> <div>76% 19%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	35	Total	C	N	O	P	1	0	0
			715	346	125	210	34			

- Molecule 2 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	34	Total	C	N	O	P	1	0	0
			696	335	124	203	34			

- Molecule 3 is a protein called Recombinase CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			
3	B	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			

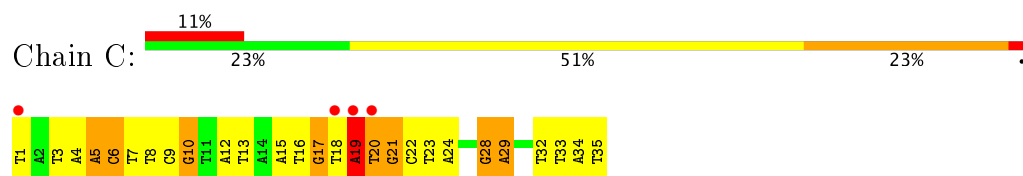
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	151	Total	O	0	0
			151	151		
4	C	35	Total	O	0	0
			35	35		
4	D	36	Total	O	0	0
			36	36		

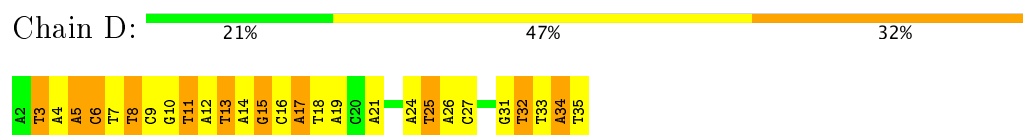
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

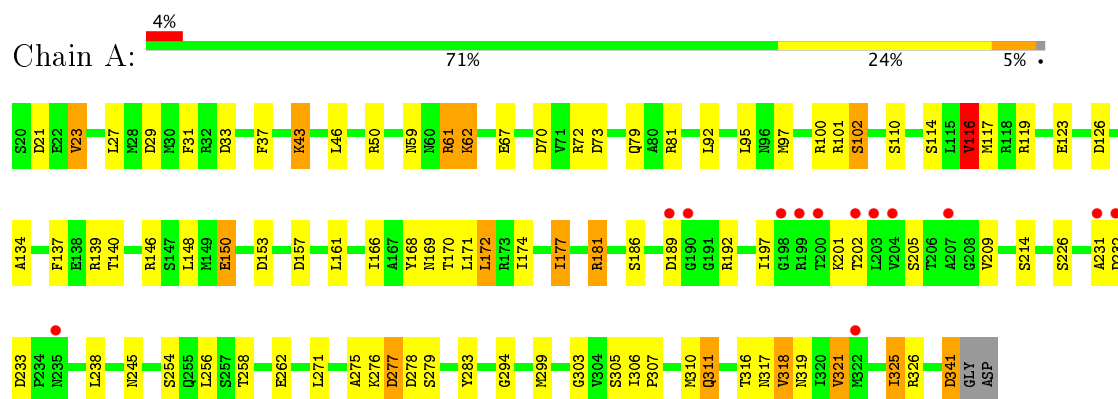
#### • Molecule 1: loxP DNA



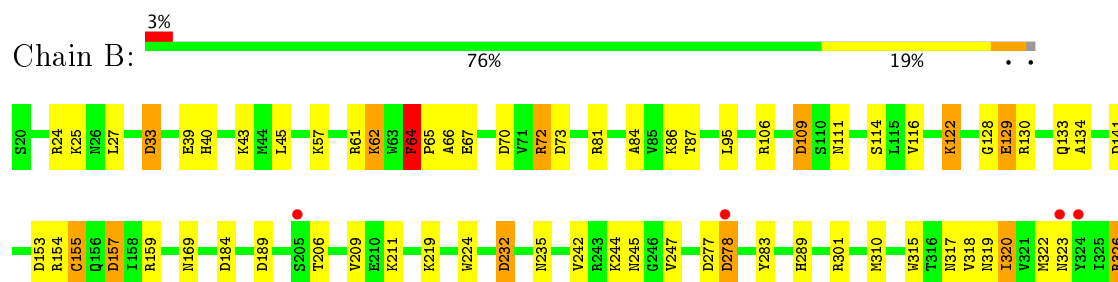
#### • Molecule 2: loxP DNA

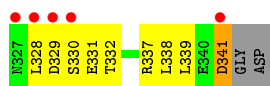


#### • Molecule 3: Recombinase CRE



#### • Molecule 3: Recombinase CRE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.08 Å   121.53 Å   177.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	47.67 – 2.80 47.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.67-2.80) 96.2 (47.60-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.196   ,   0.265 0.200   ,   0.263	Depositor DCC
$R_{free}$ test set	1386 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	1.82	6/801 (0.7%)	2.55	41/1235 (3.3%)
2	D	1.70	2/780 (0.3%)	2.20	40/1201 (3.3%)
3	A	0.60	0/2591	0.85	13/3493 (0.4%)
3	B	0.66	0/2591	0.89	14/3493 (0.4%)
All	All	1.01	8/6763 (0.1%)	1.42	108/9422 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	DT	C5-C7	32.01	1.69	1.50
2	D	18	DT	C5-C7	-28.25	1.33	1.50
1	C	19	DA	C1'-N9	-7.84	1.36	1.47
1	C	23	DT	C3'-O3'	-7.72	1.33	1.44
2	D	10	DG	C3'-O3'	-7.50	1.34	1.44
1	C	18	DT	O3'-P	6.25	1.68	1.61
1	C	7	DT	C3'-O3'	-5.88	1.36	1.44
1	C	24	DA	N7-C5	-5.52	1.35	1.39

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	DT	C6-C5-C7	-30.18	104.80	122.90
1	C	19	DA	O4'-C1'-N9	28.67	128.07	108.00
1	C	18	DT	C4-C5-C7	28.57	136.15	119.00
2	D	17	DA	O4'-C1'-N9	-16.14	96.70	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	13	DT	O4'-C1'-N1	12.76	116.93	108.00
1	C	5	DA	O4'-C1'-N9	11.29	115.91	108.00
1	C	4	DA	O4'-C1'-N9	-10.66	100.54	108.00
2	D	15	DG	O4'-C1'-N9	-9.70	101.21	108.00
2	D	32	DT	O4'-C1'-N1	-9.50	101.35	108.00
1	C	12	DA	O4'-C1'-N9	9.37	114.56	108.00
1	C	17	DG	P-O3'-C3'	9.34	130.91	119.70
1	C	28	DG	O4'-C1'-N9	-9.33	101.47	108.00
2	D	33	DT	O4'-C1'-N1	9.33	114.53	108.00
2	D	8	DT	O4'-C1'-N1	-8.91	101.76	108.00
2	D	19	DA	P-O3'-C3'	8.04	129.34	119.70
2	D	8	DT	N3-C4-O4	7.85	124.61	119.90
1	C	15	DA	O4'-C1'-N9	-7.70	102.61	108.00
1	C	20	DT	O4'-C4'-C3'	-7.59	101.44	106.00
1	C	6	DC	C2-N3-C4	-7.54	116.13	119.90
1	C	19	DA	C8-N9-C1'	-7.27	114.61	127.70
2	D	31	DG	N1-C6-O6	7.22	124.23	119.90
1	C	21	DG	O4'-C1'-C2'	-7.20	100.14	105.90
2	D	25	DT	C6-C5-C7	-7.16	118.61	122.90
3	A	157	ASP	CB-CG-OD2	6.97	124.58	118.30
1	C	32	DT	N3-C2-O2	-6.92	118.15	122.30
2	D	16	DC	C1'-O4'-C4'	-6.85	103.25	110.10
2	D	25	DT	C4-C5-C7	6.77	123.06	119.00
2	D	8	DT	O4'-C1'-C2'	-6.77	100.49	105.90
2	D	19	DA	O4'-C1'-N9	6.72	112.71	108.00
1	C	35	DT	O4'-C1'-C2'	-6.72	100.52	105.90
1	C	1	DT	O4'-C1'-N1	6.68	112.68	108.00
1	C	7	DT	N3-C4-O4	6.59	123.86	119.90
2	D	8	DT	C5-C4-O4	-6.58	120.29	124.90
1	C	6	DC	N3-C4-N4	-6.57	113.40	118.00
2	D	11	DT	N3-C4-O4	6.56	123.84	119.90
2	D	31	DG	C5-C6-O6	-6.56	124.66	128.60
2	D	7	DT	N3-C4-O4	6.52	123.81	119.90
2	D	5	DA	O4'-C1'-N9	6.47	112.53	108.00
3	B	73	ASP	CB-CG-OD2	6.46	124.11	118.30
1	C	23	DT	N3-C4-O4	6.40	123.74	119.90
2	D	17	DA	P-O3'-C3'	6.39	127.36	119.70
3	B	141	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	5	DA	C1'-O4'-C4'	-6.30	103.80	110.10
3	B	153	ASP	CB-CG-OD2	6.27	123.94	118.30
2	D	9	DC	O4'-C4'-C3'	-6.18	102.03	104.50
1	C	8	DT	N3-C2-O2	-6.16	118.60	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	DT	P-O3'-C3'	6.16	127.10	119.70
1	C	3	DT	C6-C5-C7	-6.12	119.23	122.90
1	C	7	DT	C5-C4-O4	-6.10	120.63	124.90
1	C	6	DC	N3-C2-O2	-6.10	117.63	121.90
2	D	3	DT	N3-C2-O2	-6.09	118.64	122.30
1	C	10	DG	N3-C4-C5	6.03	131.62	128.60
3	B	64	PHE	N-CA-CB	6.01	121.43	110.60
3	A	29	ASP	CB-CG-OD2	6.00	123.70	118.30
3	B	232	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	34	DA	O4'-C1'-N9	-5.95	103.84	108.00
1	C	3	DT	C4-C5-C7	5.94	122.57	119.00
2	D	31	DG	C6-C5-N7	-5.93	126.84	130.40
1	C	5	DA	O4'-C1'-C2'	-5.87	101.20	105.90
3	A	126	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	19	DA	C8-N9-C4	5.87	108.15	105.80
2	D	9	DC	N1-C1'-C2'	5.83	123.67	112.60
3	A	21	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	19	DA	N9-C4-C5	-5.81	103.47	105.80
1	C	19	DA	N9-C1'-C2'	-5.80	101.58	112.60
1	C	16	DT	C1'-O4'-C4'	-5.79	104.31	110.10
1	C	10	DG	N1-C6-O6	5.77	123.36	119.90
1	C	15	DA	P-O3'-C3'	5.75	126.60	119.70
2	D	13	DT	P-O5'-C5'	-5.75	111.70	120.90
3	B	184	ASP	CB-CG-OD2	5.73	123.45	118.30
2	D	5	DA	O4'-C1'-C2'	-5.71	101.33	105.90
1	C	34	DA	O4'-C1'-C2'	-5.66	101.37	105.90
3	A	278	ASP	CB-CG-OD2	5.66	123.39	118.30
3	A	33	ASP	CB-CG-OD2	5.64	123.37	118.30
2	D	15	DG	N9-C1'-C2'	5.62	123.29	112.60
1	C	33	DT	O4'-C1'-C2'	-5.60	101.42	105.90
3	B	70	ASP	CB-CG-OD2	5.59	123.33	118.30
3	B	33	ASP	CB-CG-OD2	5.52	123.26	118.30
2	D	27	DC	C1'-O4'-C4'	-5.51	104.58	110.10
1	C	19	DA	C4-N9-C1'	5.50	136.20	126.30
3	A	153	ASP	CB-CG-OD2	5.49	123.24	118.30
2	D	21	DA	C6-N1-C2	5.47	121.88	118.60
1	C	33	DT	C4-C5-C7	5.41	122.25	119.00
3	B	72	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	D	7	DT	C5-C4-O4	-5.37	121.14	124.90
3	B	157	ASP	CB-CG-OD2	5.37	123.13	118.30
2	D	18	DT	C5-C4-O4	-5.36	121.15	124.90
2	D	8	DT	N1-C1'-C2'	5.36	122.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	DT	C6-C5-C7	-5.33	119.70	122.90
2	D	26	DA	C2-N3-C4	5.32	113.26	110.60
1	C	29	DA	O4'-C1'-N9	5.31	111.72	108.00
3	A	116	VAL	CB-CA-C	-5.31	101.30	111.40
2	D	9	DC	C1'-O4'-C4'	-5.28	104.82	110.10
3	A	277	ASP	CB-CG-OD2	5.28	123.05	118.30
3	A	73	ASP	CB-CG-OD2	5.26	123.03	118.30
3	B	341	ASP	CB-CG-OD2	5.25	123.02	118.30
2	D	11	DT	N3-C4-C5	-5.22	112.06	115.20
2	D	34	DA	N9-C4-C5	5.22	107.89	105.80
3	A	341	ASP	CB-CG-OD2	5.20	122.98	118.30
3	A	189	ASP	CB-CG-OD2	5.17	122.95	118.30
3	A	70	ASP	CB-CG-OD2	5.13	122.91	118.30
3	B	109	ASP	CB-CG-OD2	5.13	122.91	118.30
2	D	6	DC	N1-C1'-C2'	5.11	122.32	112.60
2	D	18	DT	C4-C5-C7	-5.11	115.93	119.00
2	D	18	DT	C6-C5-C7	5.09	125.95	122.90
3	B	189	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	3	DT	O4'-C1'-N1	5.04	111.53	108.00
3	B	278	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	19	DA	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	715	0	401	10	0
2	D	696	0	387	13	0
3	A	2550	0	2571	37	0
3	B	2550	0	2571	37	0
4	A	74	0	0	3	0
4	B	151	0	0	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	0	2	1
4	D	36	0	0	5	0
All	All	6807	0	5930	90	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:DA:H2''	1:C:20:DT:O5'	1.35	1.09
3:B:67:GLU:HG3	4:B:436:HOH:O	1.62	0.97
3:A:311:GLN:HG3	4:B:487:HOH:O	1.67	0.93
3:B:64:PHE:O	3:B:65:PRO:C	2.12	0.85
3:A:31:PHE:HB2	4:A:380:HOH:O	1.79	0.83
3:B:64:PHE:O	3:B:66:ALA:N	2.17	0.77
1:C:17:DG:O6	4:C:53:HOH:O	2.04	0.73
3:B:317:ASN:OD1	3:B:319:ASN:ND2	2.20	0.73
3:B:332:THR:HG21	4:B:487:HOH:O	1.90	0.70
1:C:19:DA:H2''	1:C:20:DT:C5'	2.21	0.70
3:B:235:ASN:HB2	4:B:485:HOH:O	1.95	0.67
2:D:32:DT:O4	4:D:43:HOH:O	2.11	0.65
2:D:35:DT:O2	3:B:244:LYS:NZ	2.26	0.64
3:A:43:LYS:NZ	3:A:50:ARG:HH22	1.97	0.63
1:C:9:DC:H2''	1:C:10:DG:C8	2.35	0.62
3:B:84:ALA:O	3:B:87:THR:HG22	2.02	0.59
1:C:19:DA:C2'	1:C:20:DT:O5'	2.29	0.59
3:A:181:ARG:NH2	4:A:353:HOH:O	2.37	0.58
1:C:22:DC:OP1	4:C:42:HOH:O	2.16	0.57
3:A:119:ARG:O	3:A:123:GLU:HB2	2.04	0.56
3:A:214:SER:OG	3:B:339:LEU:HD13	2.06	0.56
3:A:43:LYS:HZ1	3:A:50:ARG:HH22	1.52	0.56
3:A:311:GLN:HB2	4:B:484:HOH:O	2.06	0.55
3:B:323:ASN:C	3:B:326:ARG:HB2	2.27	0.55
1:C:28:DG:H2''	1:C:29:DA:O5'	2.07	0.54
3:A:202:THR:OG1	3:A:205:SER:HB2	2.08	0.54
2:D:24:DA:H2'	2:D:25:DT:C6	2.43	0.54
3:A:174:ILE:HD12	3:A:258:THR:HB	1.89	0.54
2:D:3:DT:H2''	2:D:4:DA:C8	2.44	0.53
3:B:245:ASN:OD1	3:B:247:VAL:HG23	2.09	0.52
3:B:62:LYS:HB3	4:B:419:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:170:THR:OG1	3:A:172:LEU:HB2	2.10	0.52
1:C:20:DT:H2"	1:C:21:DG:C8	2.44	0.52
3:B:326:ARG:HA	4:B:448:HOH:O	2.08	0.52
3:A:101:ARG:HH11	3:B:111:ASN:HD22	1.57	0.51
3:B:155:CYS:HB3	3:B:242:VAL:HG11	1.91	0.51
3:B:72:ARG:HG3	3:B:116:VAL:HG11	1.91	0.51
3:B:81:ARG:NH1	4:B:391:HOH:O	2.43	0.51
3:B:341:ASP:HB3	4:B:474:HOH:O	2.11	0.51
3:B:328:LEU:O	3:B:330:SER:N	2.44	0.50
3:B:318:VAL:O	3:B:322:MET:HG2	2.12	0.50
2:D:12:DA:H2"	2:D:13:DT:H5"	1.94	0.49
3:A:101:ARG:HH11	3:B:111:ASN:ND2	2.11	0.48
3:A:166:ILE:HG22	3:A:177:ILE:HD13	1.96	0.48
3:B:320:ILE:HA	3:B:323:ASN:HB2	1.95	0.48
3:A:202:THR:OG1	3:A:205:SER:CB	2.62	0.48
3:B:64:PHE:HB3	3:B:65:PRO:HD3	1.96	0.47
3:B:128:GLY:O	3:B:129:GLU:C	2.53	0.47
3:B:310:MET:HB3	3:B:315:TRP:O	2.15	0.46
3:B:326:ARG:N	4:B:448:HOH:O	2.48	0.46
3:A:139:ARG:HB2	3:A:168:TYR:OH	2.16	0.46
2:D:12:DA:OP1	3:A:81:ARG:NH2	2.48	0.46
3:A:79:GLN:HB3	4:A:409:HOH:O	2.15	0.45
3:B:154:ARG:HD3	3:B:157:ASP:OD2	2.16	0.45
1:C:5:DA:H2"	1:C:6:DC:H5"	1.98	0.45
3:A:310:MET:SD	3:A:318:VAL:HG13	2.57	0.44
3:A:170:THR:O	3:A:171:LEU:C	2.55	0.44
3:B:57:LYS:HD3	4:B:489:HOH:O	2.18	0.44
3:A:146:ARG:O	3:A:150:GLU:N	2.52	0.43
3:A:245:ASN:H	3:A:245:ASN:ND2	2.16	0.43
3:A:170:THR:HB	3:A:172:LEU:HD13	1.99	0.43
3:A:59:ASN:O	3:A:61:ARG:HD3	2.19	0.43
2:D:8:DT:P	4:D:52:HOH:O	2.76	0.43
3:A:306:ILE:HB	3:A:307:PRO:HD3	2.00	0.43
3:B:159:ARG:HB2	3:B:224:TRP:CZ3	2.54	0.43
3:A:72:ARG:HG3	3:A:116:VAL:HG21	2.01	0.42
3:A:62:LYS:HD3	3:A:67:GLU:OE2	2.18	0.42
3:B:33:ASP:HA	4:B:362:HOH:O	2.19	0.42
3:A:231:ALA:O	3:A:233:ASP:N	2.52	0.42
3:A:137:PHE:O	3:A:294:GLY:HA3	2.20	0.42
1:C:21:DG:N2	2:D:17:DA:C2	2.88	0.42
2:D:14:DA:C2	2:D:15:DG:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:235:ASN:CB	4:B:485:HOH:O	2.61	0.42
2:D:11:DT:H2"	4:D:59:HOH:O	2.20	0.42
3:A:23:VAL:HB	3:A:102:SER:HB3	2.02	0.41
3:A:134:ALA:HA	3:A:283:TYR:CD1	2.56	0.41
3:A:37:PHE:C	3:B:122:LYS:HZ2	2.23	0.41
3:A:170:THR:O	3:A:172:LEU:N	2.54	0.41
3:A:62:LYS:H	3:A:62:LYS:CD	2.34	0.41
3:B:326:ARG:CA	4:B:448:HOH:O	2.67	0.41
3:A:321:VAL:O	3:A:325:ILE:HD13	2.20	0.41
2:D:32:DT:H2'	4:D:68:HOH:O	2.21	0.41
2:D:5:DA:H2"	2:D:6:DC:H5"	2.02	0.41
3:A:166:ILE:O	3:A:170:THR:HG23	2.21	0.40
4:D:67:HOH:O	3:B:40:HIS:HE1	2.05	0.40
3:A:62:LYS:HD2	3:A:62:LYS:N	2.36	0.40
3:B:106:ARG:O	3:B:109:ASP:HB2	2.21	0.40
3:B:134:ALA:HA	3:B:283:TYR:CD1	2.55	0.40
3:B:39:GLU:HG2	3:B:40:HIS:N	2.36	0.40
2:D:34:DA:C2	2:D:35:DT:C2	3.10	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:39:HOH:O	4:B:365:HOH:O[4_555]	1.80	0.40

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	320/324 (99%)	277 (87%)	38 (12%)	5 (2%)	11	36
3	B	320/324 (99%)	305 (95%)	10 (3%)	5 (2%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	640/648 (99%)	582 (91%)	48 (8%)	10 (2%)	11	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	317	ASN
3	B	64	PHE
3	B	329	ASP
3	A	232	ASP
3	A	275	ALA
3	B	232	ASP
3	A	192	ARG
3	B	326	ARG
3	A	303	GLY
3	B	277	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	269/270 (100%)	223 (83%)	46 (17%)	2	7
3	B	269/270 (100%)	242 (90%)	27 (10%)	9	26
All	All	538/540 (100%)	465 (86%)	73 (14%)	4	13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	23	VAL
3	A	27	LEU
3	A	43	LYS
3	A	46	LEU
3	A	61	ARG
3	A	62	LYS
3	A	92	LEU
3	A	95	LEU

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Mol	Chain	Res	Type
3	A	97	MET
3	A	100	ARG
3	A	102	SER
3	A	110	SER
3	A	114	SER
3	A	116	VAL
3	A	117	MET
3	A	140	THR
3	A	148	LEU
3	A	150	GLU
3	A	161	LEU
3	A	169	ASN
3	A	172	LEU
3	A	177	ILE
3	A	181	ARG
3	A	186	SER
3	A	197	ILE
3	A	201	LYS
3	A	209	VAL
3	A	226	SER
3	A	238	LEU
3	A	254	SER
3	A	256	LEU
3	A	262	GLU
3	A	271	LEU
3	A	276	LYS
3	A	277	ASP
3	A	279	SER
3	A	299	MET
3	A	305	SER
3	A	311	GLN
3	A	316	THR
3	A	318	VAL
3	A	319	ASN
3	A	321	VAL
3	A	325	ILE
3	A	326	ARG
3	A	341	ASP
3	B	24	ARG
3	B	25	LYS
3	B	27	LEU
3	B	43	LYS

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Mol	Chain	Res	Type
3	B	45	LEU
3	B	61	ARG
3	B	62	LYS
3	B	86	LYS
3	B	95	LEU
3	B	114	SER
3	B	122	LYS
3	B	129	GLU
3	B	130	ARG
3	B	133	GLN
3	B	155	CYS
3	B	169	ASN
3	B	206	THR
3	B	209	VAL
3	B	211	LYS
3	B	219	LYS
3	B	278	ASP
3	B	289	HIS
3	B	301	ARG
3	B	320	ILE
3	B	331	GLU
3	B	337	ARG
3	B	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	89	GLN
3	A	245	ASN
3	A	311	GLN
3	B	89	GLN
3	B	111	ASN
3	B	133	GLN
3	B	281	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	35/35 (100%)	0.01	4 (11%) 6 3	24, 44, 139, 182	0
2	D	34/34 (100%)	-0.51	0 100 100	26, 41, 91, 111	0
3	A	322/324 (99%)	0.08	13 (4%) 39 28	33, 60, 107, 122	0
3	B	322/324 (99%)	-0.21	9 (2%) 53 43	25, 43, 91, 121	0
All	All	713/717 (99%)	-0.08	26 (3%) 43 32	24, 51, 103, 182	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	DA	5.2
3	A	198	GLY	5.0
3	A	199	ARG	4.4
1	C	18	DT	3.8
3	A	207	ALA	3.5
1	C	1	DT	3.3
3	A	232	ASP	3.1
3	A	200	THR	3.0
3	A	202	THR	2.9
3	B	327	ASN	2.6
3	A	203	LEU	2.5
3	A	204	VAL	2.5
3	A	189	ASP	2.5
3	B	329	ASP	2.4
3	B	328	LEU	2.4
3	A	190	GLY	2.4
3	A	231	ALA	2.3
1	C	20	DT	2.2
3	B	205	SER	2.2
3	B	330	SER	2.1
3	A	235	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	341	ASP	2.0
3	B	324	TYR	2.0
3	A	322	MET	2.0
3	B	278	ASP	2.0
3	B	323	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.